

Soliton solution for particle in one-dimensional box

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A new analytical solution for particle in a one dimension box is presented in this study. The solution is derived by doing a non-linear transform to the linear schrödinger equation and converting it into Burger like equation. We obtained an interesting non-stationary wave function where our soliton solution moves in time while maintaining its shape. The resulting analytical solution exhibits several interesting features including different values of quantized velocity for real and imaginary parts of the wave function, the time-dependent expectation value of the position and $\Delta x \Delta p$. The analytical soliton solution that has been proposed, in our opinion, makes an important contribution to the study of quantum mechanics and we believe it will help us better understand how particles behave in one-dimensional box potentials.

I. INTRODUCTION

Particle in a one-dimension box is a fundamental problem in quantum mechanics, where a particle is confined in a one-dimensional box with infinite potential walls at both sides [1–9]. Despite its simplicity, the one-dimensional box potential has important applications in a range of fields, including condensed matter physics, semiconductor electronics, and quantum information science [10–17]. The solution for any quantum mechanical system can be modelled by stationary or non-stationary solution, while being entirely different in nature both play an important role in quantum physics [18, 19]. While all observables in stationary states are independent of time, in non-stationary states, the value of observables changes over time [8, 9]. In recent years, there has been growing interest in the study of soliton solutions in quantum mechanical systems [20–27]. Solitons are localized wave packets that maintain their shape and speed over long distances due to a balance between nonlinear and dispersive effects, making them particularly interesting for applications in quantum computing, communication, and information processing [28–34]. In the context of quantum mechanics, solitons are solutions to the schrödinger equation that behave as stable, self-reinforcing structures and also they are highly stable and robust, which makes them promising candidates for encoding and transmitting information in quantum systems [35, 36]. Solitons are often used as models for physical phenomena such as topological defects and quantum vortices [39–41], and they can provide insights into the behaviour of systems ranging from superfluids [42–47] to high-energy physics [48–50].

Recently, scientists have shifted to investigating solitons in the context of particles contained within a one-dimensional box [37, 38]. This is due to the one-dimensional box's role as a model system for various physical and chemical processes, such as molecules' and nanoparticles' behaviour and quantum confinement effects [51, 52]. While soliton solutions have been studied extensively in classical systems [54–57], their existence and properties in quantum mechanical systems are still an active area of research. Research has also shown that quantum soliton can be used as a quantum qubit for quantum information, quantum computing and quantum logic gates, etc [53].

In this paper, in sec II we give a new analytical solution for the same problem, where we convert the linear schrödinger equation for the flat potential into a non-linear Burger-like equation [58–60, 64] by using a few non-linear transformations. After that, we will do the inverse transformation and get the soliton solution for a particle in a one-dimension box problem. Subsequently, we will be dividing this section into further subsections, where we will apply the boundary conditions for $t = 0$ and $t \neq 0$ and calculate the average value of energy, position and momentum for our solution. In sec III we will be plotting our new results and discussing them in detail. The summary and conclusion will be discussed in sec IV.

II. FORMALISM

Here, the linear Schrödinger equation for a particle in a one-dimensional box will be changed to a nonlinear one in order to find a new analytical solution to the problem. The time-dependent Schrodinger equation for particle in the one-D box is given by,

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} = i\hbar \frac{\partial \psi(x, t)}{\partial t} \quad (1)$$

to simplify this expression let put $K = \frac{i\hbar}{2m}$, now the above equation will get reduced to the following form,

$$K \frac{\partial^2 \psi(x, t)}{\partial x^2} = \frac{\partial \psi(x, t)}{\partial t}. \quad (2)$$

We shall now perform the following non-linear transformation,

$$\psi(x, t) = e^{\alpha \phi} \quad (3)$$

where $\alpha = -1/2K$ and $\phi = \phi(x, t)$. Now by the chain rule, we can write

$$\frac{\partial \psi}{\partial t} = \alpha \frac{\partial \phi}{\partial t} e^{\alpha \phi}. \quad (4)$$

$$\frac{\partial \psi}{\partial x} = \alpha \frac{\partial \phi}{\partial x} e^{\alpha \phi}. \quad (5)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \left[\alpha \frac{\partial^2 \phi}{\partial x^2} + \alpha^2 \left(\frac{\partial \phi}{\partial x} \right)^2 \right] e^{\alpha \phi}. \quad (6)$$

Now, Eq. (1) can be written as follows utilising the results from the previous,

$$\frac{\partial \phi}{\partial t} = K \frac{\partial^2 \phi}{\partial x^2} + K \alpha \left(\frac{\partial \phi}{\partial x} \right)^2 \quad (7)$$

on differentiating the above equation with x and putting $\frac{\partial \phi}{\partial x} = u$, we will get the following,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - K \frac{\partial^2 u}{\partial x^2} = 0 \quad (8)$$

which is Burger's equation. To calculate the travelling solution of this non-linear equation, let's assume $u = u(\theta) = u(x - vt)$. Here u is to be determined. We won't solve Burger's problem again because the travelling solution is well-known in the literature already. The solution of the travelling Burger's equation is given by the following expression[64],

$$u(x, t) = \frac{u_1 + u_2 \exp(k_0(x - vt))}{1 + \exp(k_0(x - vt))} \quad (9)$$

where $u_1 = v + \sqrt{v^2 + 2A}$, $u_2 = v - \sqrt{v^2 + 2A}$ and $k_0 = \frac{u_1 - u_2}{2K}$, here A is a integration constant. Now, we will do the inverse transformation. Since

$$\frac{\partial \phi(x, t)}{\partial x} = u(x, t). \quad (10)$$

This implies

$$\phi(x, t) = \int \frac{u_1}{1 + \exp(k_0(x - vt))} dx + \int \frac{u_2 \exp(k_0(x - vt))}{1 + \exp(k_0(x - vt))} dx. \quad (11)$$

On solving this, we will get,

$$\phi(x, t) = -\frac{u_1}{k_0} \log |1 + \exp(-k_0(x - vt))| + \frac{u_2}{k_0} \log |1 + \exp(k_0(x - vt))| + \log B. \quad (12)$$

Where B is another integration constant. From eq(3), we will get

$$\psi(x, t) = \frac{B(1 + \exp(-k_0(x - vt)))^{\frac{u_1}{u_1 - u_2}}}{(1 + \exp(k_0(x - vt)))^{\frac{u_2}{u_1 - u_2}}}. \quad (13)$$

Only when $A = 0$ does the Eq. (13) satisfy the first linear Schrodinger Eq (1), which gives us $u_1 = 2v$ and $u_2 = 0$, On putting these values of u_1 and u_2 , our wave function will become

$$\psi(x, t) = B \left(1 + \exp \left(\frac{i2mv}{\hbar} (x - vt) \right) \right). \quad (14)$$

This is our new analytical solution for the wave function in particle in one-dimensional box potential. Please note that this is a travelling solution, unlike the available result in the literature for one-dimensional potential which is stationary [1-9].

A. Solution for $t = 0$

The above solution Eq. (14) has to satisfy the boundary conditions of the one-dimensional box potential at $t = 0$. So, we will apply the boundary condition at time $t = 0$ for a particle in the one-dimensional box at $x = -L/2$ and $x = L/2$, which means $\psi(-L/2, 0) = \psi(L/2, 0) = 0$

$$0 = B \left(1 + \exp \left(\frac{i2mv}{\hbar} (-L/2) \right) \right). \quad (15)$$

$$0 = B \left(1 + \exp \left(\frac{i2mv}{\hbar} (L/2) \right) \right). \quad (16)$$

Since our wave function is complex, both the real and imaginary parts of the wave function must satisfy the boundary condition separately. This gives us two different values for real and imaginary parts. For the real part,

$$v = \frac{(2n + 1)\pi\hbar}{mL}. \quad (17)$$

For the imaginary part,

$$v = \frac{n\pi\hbar}{mL}. \quad (18)$$

The total wave function will become,

$$\psi(x, 0) = B \left(1 + \cos \left(2(2n + 1) \frac{\pi x}{L} \right) + i \sin \left(2n \frac{\pi x}{L} \right) \right). \quad (19)$$

After normalising, this wave function becomes,

$$\psi(x, 0) = \frac{1}{\sqrt{2L}} \left(1 + \cos \left(2(2n + 1) \frac{\pi x}{L} \right) + i \sin \left(2n \frac{\pi x}{L} \right) \right). \quad (20)$$

The average energy of the particle will be given by the following expression,

$$E = \frac{\pi^2 \hbar^2 (5n^2 + 4n + 1)}{2mL^2}. \quad (21)$$

The average momentum of the particle is zero, which is as same as the normal particle in the one-D box result.

B. Solution for $t \neq 0$

The Eq. (14) also has to satisfy the boundary conditions of the one- dimensional box potential at $t \neq 0$. When we apply boundary condition at any time $t \neq 0$, which means

$$\psi(-L/2, t) = \psi(L/2, t) = 0$$

$$0 = B \left(1 + \exp \left(\frac{\iota 2mv}{\hbar} (-L/2 - vt) \right) \right). \quad (22)$$

$$0 = B \left(1 + \exp \left(\frac{\iota 2mv}{\hbar} (L/2 - vt) \right) \right). \quad (23)$$

On equating real parts, we get

$$-1 = \cos \frac{2mv}{\hbar} (-L/2 - vt). \quad (24)$$

$$-1 = \cos \frac{2mv}{\hbar} (L/2 - vt). \quad (25)$$

Using $\cos(-\theta) = \cos(\theta)$, the above term further simplifies to

$$(2n+1)\pi = \frac{2mv}{\hbar} (L/2 + vt). \quad (26)$$

$$(2n+1)\pi = \frac{2mv}{\hbar} (L/2 - vt). \quad (27)$$

On equating imaginary parts, we get

$$0 = \sin \frac{2mv}{\hbar} (-L/2 - vt). \quad (28)$$

$$0 = \sin \frac{2mv}{\hbar} (L/2 - vt). \quad (29)$$

Using $\sin(-\theta) = -\sin(\theta)$ will give us $0 = \sin \frac{2mv}{\hbar} (L/2 + vt)$, subsequently, the above term further simplifies to

$$n\pi = \frac{2mv}{\hbar} (L/2 + vt). \quad (30)$$

$$n\pi = \frac{2mv}{\hbar} (L/2 - vt). \quad (31)$$

On adding Eq.(26),(27) and Eq.(30),(31), we will get for the real part,

$$v = \frac{(2n+1)\pi\hbar}{mL}. \quad (32)$$

For the imaginary part,

$$v = \frac{n\pi\hbar}{mL}. \quad (33)$$

Please note here that the value of velocity that we got from applying the boundary condition at $t \neq 0$ is the same as the values for $t = 0$. Now on putting these values of velocities into Eq. (14), we will get

$$\psi(x, t) = B \left(1 + \cos \left(2(2n+1) \frac{\pi}{L} \left(x - (2n+1) \frac{\pi\hbar}{mL} t \right) \right) + \iota \sin \left(2n \frac{\pi}{L} \left(x - n \frac{\pi\hbar}{mL} t \right) \right) \right). \quad (34)$$

On normalisation, the above wave function becomes,

$$\psi(x, t) = \frac{1}{\sqrt{2L}} \left(1 + \cos \left(2(2n+1) \frac{\pi}{L} \left(x - (2n+1) \frac{\pi \hbar}{mL} t \right) \right) + i \sin \left(2n \frac{\pi}{L} \left(x - n \frac{\pi \hbar}{mL} t \right) \right) \right). \quad (35)$$

Above wave function represents a non-stationary state. The real value of the average energy of this wave function is the same as Eq. (21) because our non-stationary state is a superposition of two stationary states, the energy is time-independent even though the state is non-stationary. This means that the time dependence term gets cancelled out in the calculation of average energy. The average momentum of the particle is zero as same as for the $t = 0$ case. The average position of the particle is given by the following expression,

$$\langle x \rangle = \frac{L \sin \left(\frac{4\pi^2 n^2 \hbar t}{L^2 m} \right)}{16\pi n} + \frac{L \sin \left(\frac{2\pi^2 (2n+1)^2 \hbar t}{L^2 m} \right)}{2\pi(2n+1)} - \frac{L \sin \left(\frac{4\pi^2 (2n+1)^2 \hbar t}{L^2 m} \right)}{16\pi(2n+1)}. \quad (36)$$

It is clear from the above expression of the average position that it is time-dependent. In the next section, we will be seeing in detail how this time dependency works.

III. RESULTS AND DISCUSSIONS

In this section, we plot both the real and imaginary parts of the time-dependent wave function and analyze it for different quantum numbers at different times. Fig. 1(a) shows the real part of the wave function in Eq. (20) for quantum numbers $n = 1, 2$ and 3 , as you can see, as the number of nodes increases with increasing quantum number. The interesting fact to note here is that the number of nodes we got here differs from what we get from the existing particle solution in a one-dimensional box. From Fig. 1(b) the imaginary part of the wave function in Eq. (20) for quantum numbers $n = 1, 2$ and 3 and here also, the number of nodes increases with increasing quantum number. In Fig. 2(a) the real part of the wave function in Eq. (35) for different quantum numbers and how it progresses with time. The real part at $t = 0$ is represented by the red curve, the real part at $t = 2.5$ is represented by the black dashed curve, and the real part at $t = 5$ is represented by the blue dotted curve. Similarly in Fig. 2(b) the imaginary part of the wave function in Eq. (35) is being plotted. We can see how the wave function progresses in time for different quantum numbers. As you can see in Fig. 2 our solution maintains its shape while travelling in time. It is unusual that as our solution progresses in time, it doesn't vanish at the box's boundaries. It's because while applying boundary condition for $t \neq 0$ the time-dependent term i.e. vt gets cancelled out, so the quantized velocity we get is time-independent.

We can see how the probability distribution evolves with time (See Fig. 3). The red curve represents $t = 0$, the black dashed curve is for $t = 2$ and the blue dotted shows $t = 4$. The most crucial characteristic of a soliton is the ability to keep its shape over time while moving across space, and as you can see in the case of our soliton result the probability distribution doesn't spread out with time, it maintains its shape over time while moving only in space. The expectation value of position change with time for $t \neq 0$ case (See Fig. 4(a)). The quantity $\Delta x \Delta p$ is also plotted with time (See Fig. 4(b)), where Δx represents the uncertainty in the measurement of position and similarly Δp represents the uncertainty in the measurement of momentum.

IV. CONCLUSION

In conclusion, we have given a new solution for the well-known problem, particle in a one-D box. This new analytical solution displays extraordinary behaviour in terms of maintaining its shape while moving. Also, we saw how the average value of position changes with time, which implies that our wave function for particle in one-dimensional box is not stationary, which is not the case for the already established result of particle in one-dimensional box. The results of this work are applicable to several one-dimensional physical systems such as carbon nanotubes, quantum dots, and semiconductor nanowires. The analytical soliton solution described here sheds light on both the behaviour of restricted systems and the fundamental properties of quantum physics. Overall, the findings of this work help advance our understanding of the intricate behaviour of quantum mechanical systems. The analytical soliton solution provided in this publication lays the groundwork for additional research into restricted systems and could result in quantum mechanical advancements in the future.

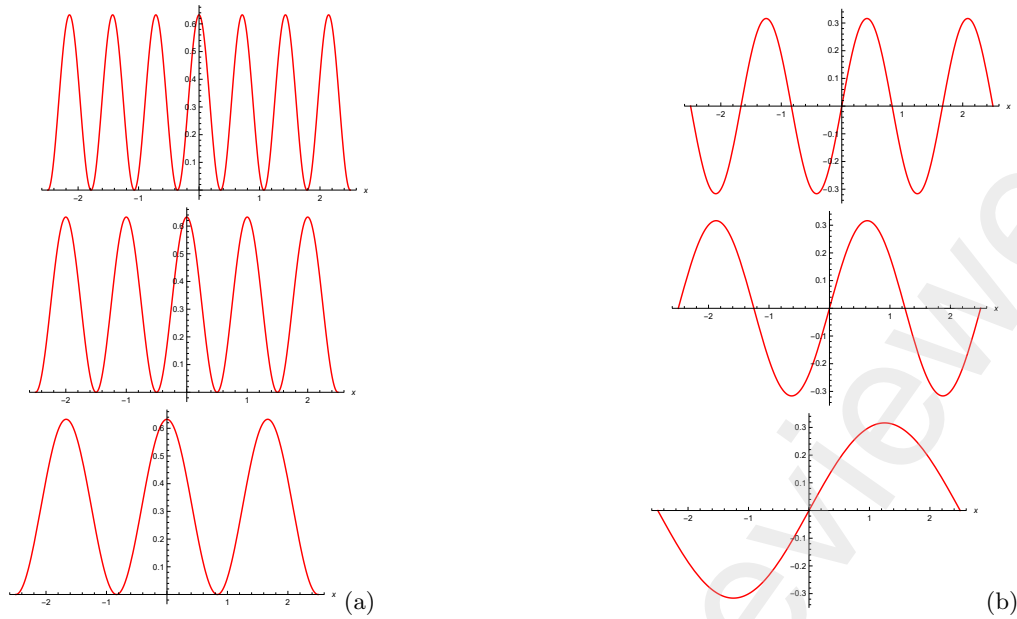


FIG. 1: Plot of the real and imaginary part of the wave function for different quantum numbers. Fig[a] represents the Real part of the wave function for quantum numbers $n=1,2$ and 3 at time $t = 0$. Fig [b] represents the imaginary part of the wave function for quantum numbers $n=1,2$ and 3 at time $t = 0$. For $L = 5, m = 1$ and $\hbar = 1$

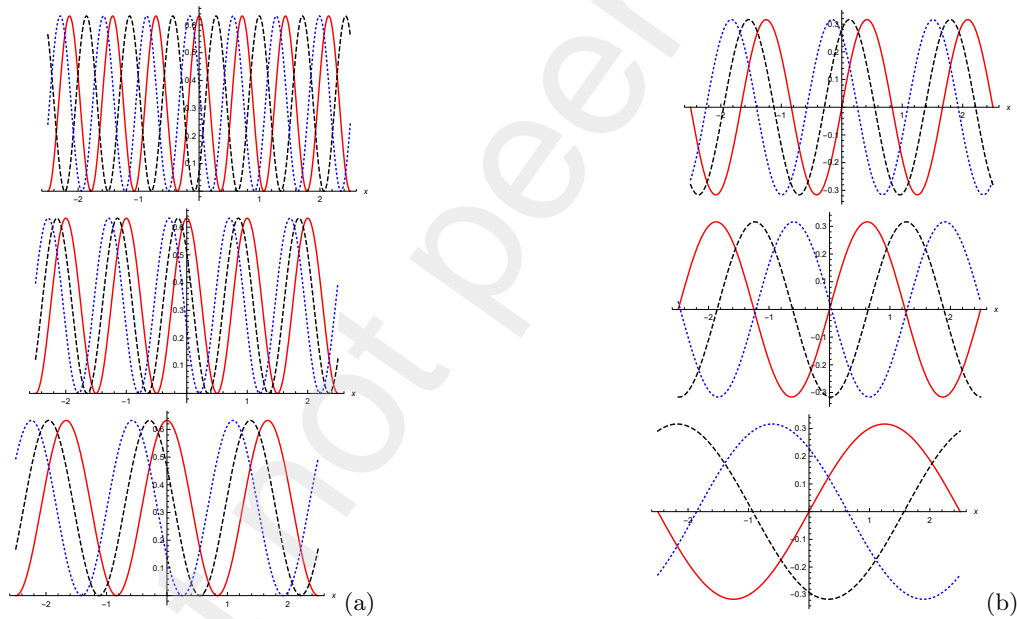


FIG. 2: Plot of the real and imaginary part of the wave function for different quantum numbers at different times. Fig[a] represents the Real part of the wave function for quantum numbers $n=1,2$ and 3 at time $t = 0$ (Red), $t = 2.5$ (Black, Dashed) and $t = 5$ (Blue, Dotted). Fig [b] represents the imaginary part of the wave function for quantum numbers $n=1,2$ and 3 at time $t = 0$ (Red), $t = 2.5$ (Black, Dashed) and $t = 5$ (Blue, Dotted). For $L = 5, m = 1$ and $\hbar = 1$

V. DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper

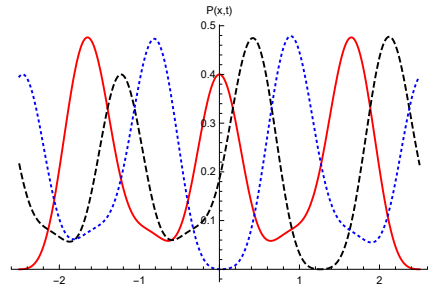


FIG. 3: The plot of the probability distribution vs position at different times. The length of the box is $L = 5$. and is plotted for quantum number $n = 1$. We have set $\hbar = 1$ and $m = 1$. Here the red curve represents $t = 0$, the black dashed curve is for $t = 2$ and the blue dotted shows $t = 4$.

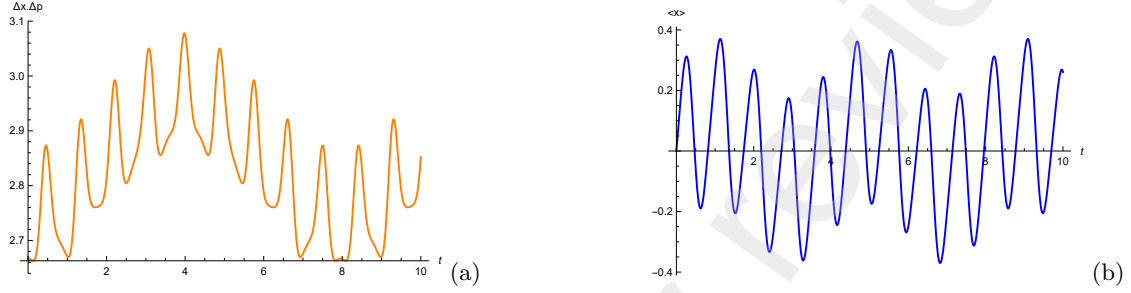


FIG. 4: Plot of the uncertainty in position and momentum vs time (a) and the average position vs time (b). The length of the box is $L = 5$. and is plotted for quantum number $n = 1$. We have set $\hbar = 1$ and $m = 1$

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